

UNIVERSITI SAINS MALAYSIA

Second Semester Examination  
2010/2011 Academic Session

April/May 2011

**EKC 245 – Mathematical Methods For Chemical Engineering**  
***[Kaedah Matematik Kejuruteraan Kimia]***

Duration : 3 hours  
*[Masa : 3 jam]*

Please ensure that this examination paper contains SIX printed pages and THREE printed page of Appendix before you begin the examination.

*[Sila pastikan bahawa kertas peperiksaan ini mengandungi ENAM muka surat yang bercetak dan TIGA muka surat Lampiran sebelum anda memulakan peperiksaan ini.]*

**Instruction:** Answer **ALL** questions.

**[Arahan:** Jawab **SEMUA** soalan.]

In the event of any discrepancies, the English version shall be used.

*[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah digunapakai].*

1. The concentration of biochemical oxygen demand (BOD),  $m$ , in a wastewater treatment tank decreases according to

*Kepekatan keperluan oksigen biokimia (BOD),  $m$ , di dalam tangki rawatan air sisa berkurang berdasarkan*

$$m = 75e^{-1.5t} + 20e^{-0.075t}$$

Determined the time,  $t$  required for the BOD concentration to be reduced to 15 using Newton-Raphson method with initial guess of  $t = 6$  and a stopping criterion of 0.5%. Verify your result.

*Tentukan masa,  $t$  yang diperlukan bagi mengurangkan kepekatan BOD kepada 15 dengan menggunakan kaedah Newton-Raphson, anggaran awal  $t = 6$  dan kriteria berhenti 0.5%. Buktikan keputusan anda.*

[25 marks/markah]

2. Figure Q.2. shows three reactors linked by pipes. As indicated, the rate of transfer of chemicals through each pipe is equal to a flowrate ( $Q$ , with units of cubic meters per second) multiplied by the concentration of the reactor from which the flow originates ( $c$ , with units of milligrams per cubic meter). If the system is at a steady state, the transfer into each reactor will balance the transfer out. The flowrates are given as  $Q_{13} = 20$ ,  $Q_{12} = 45$ ,  $Q_{21} = 15$ ,  $Q_{23} = 30$  and  $Q_{33} = 60$ . Develop mass-balance equations for the reactors and indentify their concentrations using

*Rajah S.2. menunjukkan tiga reaktor dihubungkan dengan paip. Seperti tertera, kadar pemindahan bahan kimia melalui setiap paip bersamaan dengan kadar alir ( $Q$ , dengan unit meter padu per saat) didarab dengan kepekatan reaktor daripada aliran asal tersebut ( $c$ , dengan unit milligram per meter padu). Jika sistem tersebut dalam keadaan mantap, pemindahan masuk ke setiap reaktor seimbang dengan pemindahan keluar. Kadar aliran diberi sebagai  $Q_{13} = 20$ ,  $Q_{12} = 45$ ,  $Q_{21} = 15$ ,  $Q_{23} = 30$  dan  $Q_{33} = 60$ . Terbitkan persamaan keseimbangan jisim untuk semua reaktor dan tentukan kepekatan masing-masing menggunakan*

[a] Gauss elimination method  
*Kaedah penyisihan Gauss*

[b] Gauss-Seidel method  
*Kaedah Gauss-Siedel*

[25 marks/markah]

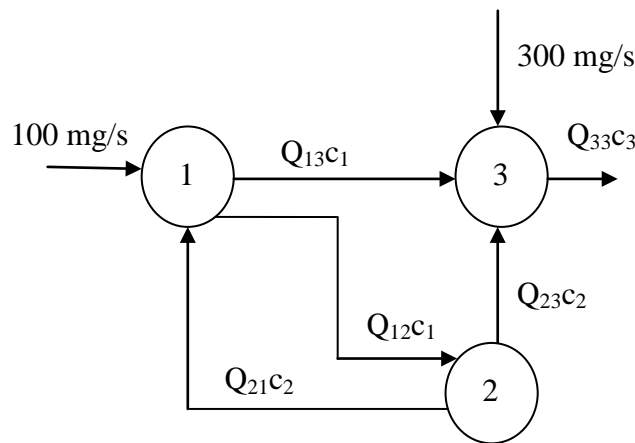


Figure Q.2.  
Rajah S.2.

3. [a] A temperature function across a board is  
*Fungsi suhu merentasi satu papan ialah*
- $$f(x,y) = 5x^2 - xy + y^2 + 3y$$
- [i] Find the maximum temperature based on analytical solution.  
*Carikan suhu maksima berdasarkan penyelesaian analitikal.*  
[6 marks/markah]
- [ii] Perform two iteration of steepest ascent method on the function starting at point (1,1).  
*Lakukan dua lelaran kaedah naik tercuram pada fungsi tersebut bermula dari titik (1,1).*  
[8 marks/markah]
- [iii] List out the advantages and disadvantages of steepest ascent/descend method.  
*Senaraikan kebaikan dan keburukan kaedah naik/turun tercuram.*  
[4 marks/markah]
- [b] Reactant A is being converted into product X in a system. The rate of reaction for each species is given as follows:  
*Bahan tindak balas A ditukar kepada produk X dalam suatu sistem. Kadar tindak balas bagi setiap spesis adalah diberi seperti di bawah:*

$$\frac{dC_A}{dt} = -k_1 C_A^2 + k_2 C_X$$

$$\frac{dC_X}{dt} = \frac{k_1 C_A^2}{1 + KC_X}$$

where  $C_i$  = concentration of species  $i$ ;  $t$  = time in s and rate constants  $k_1 = 0.514 \text{ (mol/ dm}^3\text{)}^{-1}\text{s}^{-1}$ ;  $k_2 = 0.238 \text{ s}^{-1}$ ;  $K = 0.752 \text{ (mol/ dm}^3\text{)}^{-1}$ . Find the concentration of A, and X after 1 s. The initial feed to the reactor is pure A with concentration  $2 \text{ mol/dm}^3$ .

di mana  $C_i$  = kepekatan spesis  $i$ ;  $t$  = masa dalam saat dan pemalar kadar  $k_1 = 0.514 \text{ (mol/ dm}^3\text{)}^{-1}\text{s}^{-1}$ ;  $k_2 = 0.238 \text{ s}^{-1}$ ;  $K = 0.752 \text{ (mol/ dm}^3\text{)}^{-1}$ . Carikan kepekatan A dan X selepas 1 saat. Suapan awal ke reaktor ialah A tulen dengan kepekatan  $2 \text{ mol/dm}^3$ .

[7 marks/markah]

4. [a] [i] A heated plate is subjected to two boundary temperatures held at constant value (in degree Celsius) at certain positions and two boundaries being insulated as shown in Figure Q.4.[a]. Use Liebmann's method to solve for the temperature at the nodes in the grid (calculate the temperature at 6 points) of the heated plate to compute the steady state distribution of temperature. Employ overrelaxation with a value of 1.5 for the weighting factor and iterate 1 time. Start from the point  $i = 1, j = 0$  with the assumption that all the unknown points are zeros.

Sebuah plat panas dengan dua suhu sempadan yang dikekalkan (darjah Celsius) pada suhu tetap di titik-titik tertentu dan dua sempadan ditebat adalah ditunjukkan dalam Rajah S.4.[a]. Gunakan kaedah Liebmann untuk menyelesaikan suhu di titik-titik grid (kirakan suhu bagi 6 titik) pada plat panas untuk mencari taburan suhu pada keadaan mantap. Gunakan santaian dengan nilai 1.5 bagi faktor pemberat dan lelar 1 kali. Mula dari titik  $i = 1, j = 0$  dengan anggapan bahawa semua titik anu adalah sifar.

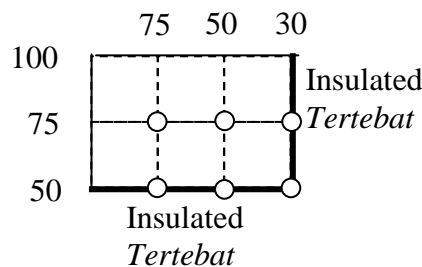


Figure Q.4.[a].  
Rajah S.4.[a].

[10 marks/markah]

- [ii] Given the temperature (in degree Celsius) distribution of a heated plate at steady state is given as shown in Figure Q.4.[b]. Calculate the fluxes for the two nodes in the grid of the plate.

*Taburan suhu (dalam darjah Celsius) bagi sebuah plat panas pada keadaan mantap adalah seperti dalam Rajah S.4.[b]. Hitungkan fluks bagi dua titik pada plat panas tersebut.*

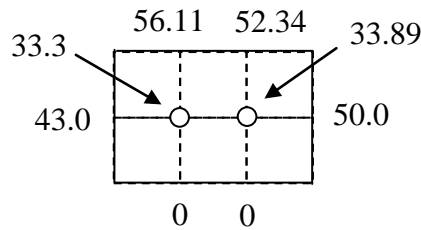


Figure Q.4.[b].  
Rajah S.4.[b].

Assume that the plate is 20 cm x 30 cm and is made out of aluminum.  
*Anggapkan plat tersebut adalah 20 sm x 30 sm dan diperbuat daripada aluminium.*

$$[k' = 0.49 \text{ cal/s.cm.}^{\circ}\text{C}]$$

Hint: Fourier's law of heat conduction:

*Petunjuk: Hukum Fourier bagi konduksi haba:*

$$q_i = -k' \frac{\partial T}{\partial i} \text{ where } q_i = \text{heat flux in the direction of the } i \text{ dimension}$$

[cal/cm<sup>2</sup>.s]

$$q_i = -k' \frac{\partial T}{\partial i} \text{ di mana } q_i = \text{fluks haba pada arah dimensi } i \text{ [cal/sm}^2\text{.s]}$$

[5 marks/markah]

- [b] A 4 cm long thin rod is insulated at all point except at its ends. At time  $t = 0$ , the temperature of the whole rod is  $30^{\circ}\text{C}$  and the boundary conditions are fixed for all times at  $T(0) = 120^{\circ}\text{C}$  and  $T(10) = 45^{\circ}\text{C}$ . Given  $\Delta x = 1 \text{ cm}$ ,  $\Delta t = 1 \text{ s}$  and  $k = 0.944 \text{ cm}^2/\text{s}$ . Calculate the temperature distribution at  $t = 1 \text{ s}$  using the simple implicit method. The Laplacian difference equations for the system is given as

*Satu rod halus yang panjangnya 4 sm ditebat pada semua titik kecuali pada kedua-dua hujungnya. Pada masa  $t = 0$ , suhu seluruh rod tersebut ialah  $30^{\circ}\text{C}$  dan keadaan sempadan dikekalkan pada  $T(0) = 120^{\circ}\text{C}$  dan  $T(10) = 45^{\circ}\text{C}$ . Diberi  $\Delta x = 1 \text{ sm}$ ,  $\Delta t = 1 \text{ s}$  dan  $k = 0.944 \text{ sm}^2/\text{s}$ . Kirakan taburan suhu pada  $t = 1 \text{ s}$  menggunakan kaedah implisit mudah. Persamaan Laplace bagi sistem tersebut diberi sebagai*

$$-\lambda T_{i-1}^{l+1} + (1 + 2\lambda)T_i^{l+1} - \lambda T_{i+1}^{l+1} = T_i^l \text{ where } \lambda = k \Delta t / (\Delta x)^2$$

[10 marks/markah]

## Appendix

### Matrix of Polynomial Regression

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{Bmatrix}$$

### Matrix of Multiple Linear Regression

$$\begin{bmatrix} n & \sum x_{1i} & \sum x_{2i} \\ \sum x_{1i} & \sum x_{1i}^2 & \sum x_{1i} x_{2i} \\ \sum x_{2i} & \sum x_{1i} x_{2i} & \sum x_{2i}^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_{1i} y_i \\ \sum x_{2i} y_i \end{Bmatrix}$$

## Differentiation Formulas

### *Forward finite-divided-difference*

$$\begin{aligned} \text{First derivative} \quad f'(x_i) &= \frac{f(x_{i+1}) - f(x_i)}{h} & O(h) \\ f'(x_i) &= \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} & O(h^2) \end{aligned}$$

$$\begin{aligned} \text{Second derivative} \quad f''(x_i) &= \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} & O(h) \\ f''(x_i) &= \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} & O(h^2) \end{aligned}$$

### *Backward finite-divided-difference*

$$\begin{aligned} \text{First derivative} \quad f'(x_i) &= \frac{f(x_i) - f(x_{i-1})}{h} & O(h) \\ f'(x_i) &= \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} & O(h^2) \end{aligned}$$

$$\begin{aligned} \text{Second derivative} \quad f''(x_i) &= \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} & O(h) \\ f''(x_i) &= \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} & O(h^2) \end{aligned}$$

### *Centred finite-divided-difference*

$$\text{First derivative} \quad f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h} \quad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2}))}{12h} \quad O(h^4)$$

$$\text{Second derivative} \quad f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{h^2} \quad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2}))}{12h^2} \quad O(h^4)$$

### *Derivatives of unequally spaced data*

$$f'(x) = f(x_{i-1}) \frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i) \frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} + f(x_{i+1}) \frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}$$

### **Integration Formulas**

#### Trapezoidal Rule

$$I = (a - b) \frac{f(a) + f(b)}{2}$$

$$I = (b - a) \frac{f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}$$

#### Simpson's 1/3 Rule

$$I \cong (b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$$

$$I \cong (b - a) \frac{f(x_0) + 4 \sum_{i=1,3,5}^{n-1} f(x_i) + 2 \sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}$$



## Useful Formula

*ODE solver*

Euler's method

$$y_{i+1} = y_i + y_i' h$$

4<sup>th</sup> order Runge-Kutta

$$y_{i+1} = y_i + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4)h$$

where  $k_1 = f(x, y)$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1h\right)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2h\right)$$

$$k_4 = f(x_i + h, y_i + k_3h)$$

*Finite difference methods*

Laplacian difference equations

$$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4 T_{i,j} = 0$$

Explicit method:

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \quad \frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{\Delta x^2}$$

Simple implicit method:

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \quad \frac{\partial^2 T}{\partial x^2} \cong \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2}$$

The Crank Nicolson Method

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \quad \frac{\partial^2 T}{\partial x^2} \cong \frac{1}{2} \left[ \frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{(\Delta x)^2} + \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2} \right]$$

Overrelaxation

$$T_{i,j}^{new} = \lambda T_{i,j}^{new} + (1 - \lambda) T_{i,j}^{old}$$